Pyridoxal, TMS

Inchi: InChI=1S/C14H25NO3Si2/c1-11-14(18-20(5,6)7)13(9-16)12(8-15-11)10-17-19(2,3)4/h8-9
InchiKey: KRAALPWVLKNYLF-UHFFFAOYSA-N
Formula: C14H25NO3Si2
SMILES: Cc1ncc(CO[Si](C)(C)C)c(C=O)c1O[Si](C)(C)C
Mol. weight [g/mol]: 311.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.24		Crippen Method
logp	3.768		Crippen Method
rinpol	1745.00		NIST Webbook
rinpol	1745.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R95313&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices